

# Refined Spectral Method as an extremely accurate technique for solving 2D time-independent Schrödinger equation

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February 7, 2008

## Abstract

We present a refinement of the Spectral Method by incorporating an optimization method into it and generalize it to two space dimensions. We then apply this Refined Spectral Method as an extremely accurate technique for finding the bound states of the two dimensional time-independent Schrödinger equation. We first illustrate the use of this method on an exactly solvable case and then use it on a case which is not so. This method is very simple to program, fast, extremely accurate (*e.g.* a relative error of  $10^{-15}$  is easily obtainable in two dimensions), very robust and stable. Most importantly, one can obtain the energies and the wave functions of as many of the bound states as desired with a single run of the algorithm.

*PACS numbers:* 02.70.Hm, 03.65.Ge

## 1 Introduction

Eighty years after the birth of quantum mechanics [1], the Schrödinger's famous equation still remains a subject for numerous studies, aiming at extending its field of applications and at developing more efficient analytic and approximation methods for obtaining its solutions. There has always been a remarkable interest in studying exactly solvable Schrödinger equations which has been found for only a very limited number of potentials, most of them being classified

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already by Infeld and Hull [2] on the basis of the Schrödinger factorization method [3], which in turn appeared to be a rediscovery of the formalism stated nearly 120 years ago by Darboux [4]. However, a vast majority of the problems of physical interest do not fall in the above category when we formulate a more or less realistic model for them. Then we have to resort to approximation techniques which can be analytic or numeric. The Schrödinger equation can always be solved numerically, which nowadays seems elementary, in view of the immensely increased computational power. However, even in this simplest case, the success of applying any direct numerical integration method depends on the quality of initial guesses for the boundary conditions and energy eigenvalues. Moreover, one usually encounters difficulties with the intrinsic instabilities of typical problems, and rarely with the existence of actual solutions which possess rapid oscillation. The need for evermore accurate and efficient numerical methods for solving problems of physical interest have stimulated development of more sophisticated integration approaches, *e.g.* embedded exponentially-fitted Runge-Kutta [5] and dissipative Numerov-type [6] methods, as well as interesting techniques, such as a relaxation approach [7] based on the Henyey algorithm [8], an adaptive basis set using a hierarchical finite element method [9], and an approach based on microgenetic algorithm [10], which is a variation of a global optimization strategy proposed by Holland [11]. Most of these methods are either completely designed for the one-dimensional cases or optimized so. Few general methods are readily available for higher dimensional cases, *e.g.* Finite Element Method (FEM), Finite Difference Method (FDM), Relaxation Method, Spectral Element Method.

Here we extend the Refined Spectral Method (RSM), which is introduced in Ref. [12], as a numerical method to solve the higher dimensional Schrödinger equations. There, we first refined the Spectral Method (SM) [13] for one-dimensional cases by incorporating an optimization procedure into it, and then tested the results obtained by our method against the corresponding values of an exactly solvable case. We showed that this method can be extremely accurate, (*e.g.* errors of order  $10^{-130}$ ), and has the following advantages: It is very simple, fast, very robust and stable, *i.e.* it does not have the instability problems due to the usual

existence of divergent solutions of most physical problems. These problems usually produce difficulties for the spatial integration routines such as FDM and FEM. Finally, and perhaps most importantly, we can obtain the wave functions and energies of as many of the bound states as desired with a single run of the algorithm. Spectral Method, consists of first choosing a complete orthonormal set of eigenstates of a, preferably relevant, hermitian operator to be used as a suitable basis for our solution. For this numerical method we obviously can not choose the whole set of the complete basis, as these are usually infinite. Therefore we make the approximation of representing the solution by a superposition of only a finite number of the basis functions. By substituting this approximate solution into the differential equation, a matrix equation is obtained. The energies and expansion coefficients of these approximate solutions could be determined by the eigenvalues and eigenfunctions of this matrix, respectively. In the Spectral Method the concentration is on the basis functions and we expect the final numerical solution to be approximately independent of the actual basis used. Moreover in this method, the refinement of the solution is accomplished by choosing a larger set of basis functions, rather than choosing more grid points, as in the numerical integration methods. For more detailed explanation on this subject, in particular different branches of SM, including the commonly used Pseudo-Spectral Method, and its historical development see for example Ref. [13]. For an interesting application of this method to the double well potential see for example Ref. [14].

The remainder of this paper is organized as follows. In Section 2, we present the underlying theoretical bases for the formulation of the RSM and introduce our optimization procedure in two-dimensions. In Section 3, we first use this method for the 2D Simple Harmonic Oscillator (2D-SHO), which is an exactly solvable problem, to illustrate and test the method. In Section 4, we apply this method to an interesting 2D problem which could be relevant to QCD and is not exactly solvable. In Section 5, we state our conclusions.

## 2 The Refined Spectral Method

Let us consider the 2-D time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \left( \frac{d^2\psi(x, y)}{dx^2} + \frac{d^2\psi(x, y)}{dy^2} \right) + U(x, y)\psi(x, y) = E\psi(x, y), \quad (1)$$

where  $m$ ,  $U(x, y)$ , and  $E$  stand for the reduced mass, potential energy, and energy, respectively. Obviously, This is an eigenvalue problem with eigenfunction  $\psi(x, y)$  and eigenvalue  $E$ . Throughout this paper, we only examine the bound states of this problem, i.e. the states which are the square integrable. Therefore the general eigenvalue problem that we want to solve can be cast in the form of a linear elliptic PDE one that can be written as,

$$-\left( \frac{d^2\psi(x, y)}{dx^2} + \frac{d^2\psi(x, y)}{dy^2} \right) + \hat{f}(x, y)\psi(x, y) = \varepsilon \psi(x, y), \quad (2)$$

where,

$$\hat{f}(x, y) = \frac{2m}{\hbar^2} U(x, y), \quad \varepsilon = \frac{2m}{\hbar^2} E. \quad (3)$$

The configuration space for most physical problems are defined by  $-\infty < x, y < \infty$ . We make the approximation of constraining the domain to  $-L_x/2 < x < L_x/2$  and  $-L_y/2 < y < L_y/2$ . As shall be explained later, first of all, this constraining of the domain is absolutely crucial for our method, and secondly does not necessarily pose a loss of accuracy: The use of a finite domain is necessary since we need to choose a finite subspace of a countably infinite basis. Moreover, since the bound states have compact support, a finite region suffices, and the choices of  $L_x$  and  $L_y$  are in fact the essential part of our optimization procedure. As mentioned before, any complete orthonormal set can be used for the SM. We use the Fourier series basis as an example. For this particular basis, we find it convenient to shift the domain to  $0 < x < L_x$  and  $0 < y < L_y$ . In particular, we need to shift the potential energy functions also. This means that we can expand the solution as,

$$\psi(x, y) = \sum_{m,n=1}^{\infty} A_{m,n} \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right). \quad (4)$$

We can also make the following expansion,

$$\hat{f}(x, y)\psi(x, y) = \sum_{m,n} B_{m,n} \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right), \quad (5)$$

where  $B_{m,n}$  are coefficients that can be determined once  $\hat{f}(x, y)$  is specified. By substituting Eqs. (4,5) into Eq. (2) and using the differential equation of the Fourier basis we obtain,

$$\sum_{m,n} \left[ \left( \left( \frac{m\pi}{L_x} \right)^2 + \left( \frac{n\pi}{L_y} \right)^2 - \varepsilon \right) A_{m,n} + B_{m,n} \right] \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right) = 0. \quad (6)$$

Because of the linear independence of  $\sin\left(\frac{m\pi x}{L_x}\right)$  and  $\sin\left(\frac{n\pi y}{L_y}\right)$ , every term in the summation must satisfy,

$$\left( \left( \frac{m\pi}{L_x} \right)^2 + \left( \frac{n\pi}{L_y} \right)^2 \right) A_{m,n} + B_{m,n} = \varepsilon A_{m,n}. \quad (7)$$

It only remains to determine the matrix  $B$ . Using Eq. (5) and Eq. (4) we have,

$$\sum_{m,n} B_{m,n} \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right) = \sum_{m,n} A_{m,n} \hat{f}(x, y) \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right). \quad (8)$$

By multiplying both sides of the above equation by  $\sin\left(\frac{m'\pi x}{L_x}\right) \sin\left(\frac{n'\pi y}{L_y}\right)$  and integrating over the  $x, y$ -space and using the orthonormality condition of the basis functions, one finds,

$$B_{m,n} = \sum_{m',n'} C_{m,m',n,n'} A_{m',n'}, \quad (9)$$

where,

$$C_{m,m',n,n'} = \left( \frac{4}{L_x L_y} \right) \int_0^{L_x} \int_0^{L_y} \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right) \hat{f}(x, y) \sin\left(\frac{m'\pi x}{L_x}\right) \sin\left(\frac{n'\pi y}{L_y}\right) dx dy. \quad (10)$$

Therefore we can rewrite Eq. (7) as,

$$\left( \left( \frac{m\pi}{L_x} \right)^2 + \left( \frac{n\pi}{L_y} \right)^2 \right) A_{m,n} + \sum_{m',n'} C_{m,m',n,n'} A_{m',n'} = \varepsilon A_{m,n}. \quad (11)$$

It is obvious that the presence of the operator  $\hat{f}(x, y)$  in Eq. (2), leads to nonzero coefficients  $C_{m,m',n,n'}$  in Eq. (11), which in principle could couple all of the matrix elements of  $A$ . It is easy to see that the more basis functions we include, the closer our solution will be to the exact

one. We select a finite subset of the basis functions *i.e.* the first  $N^2$  ones, by letting the index  $m$  and  $n$  run from 1 to  $N$  in the summations. Then we replace the square matrix  $A$  with a column vector  $A'$  with  $N^2$  elements, so that any element of  $A$  corresponds to one element of  $A'$ . With this replacement, Eq. (11) can be written as,

$$D A' = \varepsilon A', \quad (12)$$

where  $D$  is a square matrix with  $(N^2) \times (N^2)$  elements. Its elements can be obtained from Eq. (11). The eigenvalues and eigenfunctions of the Schrödinger equation are approximately equal to the corresponding quantities of the matrix  $D$ . That is the solution to this matrix equation simultaneously yields  $N^2$  sought after eigenstates and eigenvalues. The only problem which remains is to solve the eigenvalue problem Eq. (12), and to control the round-off errors. This is often a serious issue for the usual spatial integration method using double precision. However, we can easily overcome this problem and obtain a very high precision. Using RSM in 1D accuracies of order 100 significant digits are very easily accomplishable while in 2D 10 significant digits are obtained using the same computation time. This can be implemented, for instance with MATHEMATICA, using the instruction ‘Set[Precision[...],20]’, for example, to set a precision of 20 digits for the numbers. This method, in principle, allows us to obtain the eigenvalues and eigenvectors with a maximum precision of 20 digits (using enough basis elements).

Now we can introduce our optimization procedure. We are free to adjust two parameters:  $N$ , the number of basis elements used and the lengths of the spatial region,  $L_x$  and  $L_y$ . These lengths should be preferably larger than spatial spreading of all the sought after wave functions. However, if  $L_x$  and  $L_y$  are chosen to be too large we loose overall accuracy. After fixing these lengths, any desired accuracy can be obtained with a suitable choice of  $N$ . As we shall show, the error decreases extremely rapidly as the number of basis elements is increased. However, it is important to note that for each  $N$ ,  $L_x$  and  $L_y$  have to be properly adjusted. We shall denote these optimal quantities by  $\hat{L}_x(N)$  and  $\hat{L}_y(N)$ . We have come up with a method to determine

these quantities: For a few fixed values of  $N$  we compute  $E(N, L_x, L_y)$  which invariably has an minimum point. Therefore, all we have to do is to compute the position of these minimum points and compute an interpolating function for obtaining  $\hat{L}_x(N)$  and  $\hat{L}_y(N)$ . Obviously the more points we choose the better our results will be. As we shall see, the addition of this refinement can have dramatic consequences.

Computation of the relative error in the exactly solvable cases is straightforward. For example for computing the relative error of the eigenvalue, denoted by  $\delta_E$ , we only need to find the absolute value of the difference between the result and the exact one and divide by the latter. For cases which are not exactly solvable, we compute the difference between the eigenvalues for a given  $N$  and those obtained with  $N + 1$ , both lying on the  $\hat{L}_x(N)$  and  $\hat{L}_y(N)$  curves. We shall denote the error computed by this procedure  $\hat{\delta}_E$ . We have computed  $\hat{L}_x(N)$  and  $\hat{L}_y(N)$  for all cases, and subsequently computed the eigenfunctions, eigenvalues and their errors using this method, and checked their validity in the exactly solvable case of 2D-SHO. Obviously to obtain consistent results we have to keep the same precision throughout the calculations.

### 3 2D Simple Harmonic Oscillator

In this section, for illustrative purposes, we apply RSM to find the bound states of a 2D-SHO. We can then readily check the validity of our whole procedure, which includes our prescription for finding the optimal quantities  $\hat{L}_x(N)$  and  $\hat{L}_y(N)$ , and the overall accuracy of our results.

The Schrödinger equation for an isotropic 2D-SHO is,

$$-\frac{\hbar^2}{2m} \left( \frac{d^2\psi(x', y')}{dx'^2} + \frac{d^2\psi(x', y')}{dy'^2} \right) + \frac{1}{2}m\omega^2(x'^2 + y'^2)\psi(x', y') = E'\psi(x', y'), \quad (13)$$

where  $\omega$  is the natural frequency of the Oscillator. We first shift the variables as explained above, and then we convert this differential equation into the following dimensionless form by dividing both sides by  $\hbar\omega/2$ ,

$$-\frac{d^2\psi(x, y)}{dx^2} - \frac{d^2\psi(x, y)}{dy^2} + \left( (x - L_x/2)^2 + (y - L_y/2)^2 \right) \psi(x, y) = E\psi(x, y), \quad (14)$$

where  $x = \sqrt{\frac{m\omega}{\hbar}}x', y = \sqrt{\frac{m\omega}{\hbar}}y'$ , and  $E = \frac{2}{\hbar\omega}E'$ . This differential equation is exactly solvable and its eigenvalues and eigenfunctions, which are all bound states, can be easily found analytically and are well known,

$$\psi_{n_x, n_y}(x, y) = \left(\frac{1}{\pi}\right)^{1/2} \frac{H_{n_x}(x)H_{n_y}(y)}{\sqrt{2^{n_x+n_y}n_x!n_y!}} e^{-(x^2+y^2)/2}, \quad (15)$$

$$E_{n_x, n_y} = 2(n_x + n_y + 1), \quad n_x, n_y = \{0, 1, 2, \dots\}, \quad (16)$$

where  $H_n(x)$  denote the Hermite polynomials. Using RSM we can calculate accurately the energy levels and the corresponding eigenfunctions of this Hamiltonian. Here, we choose our optimization procedure for the ground state which will be symmetric in  $x$  and  $y$ , therefore  $\hat{L}_x(N) = \hat{L}_y(N) \equiv \hat{L}(N)$ . The computation of the errors of the wave functions are analogous to that of the energy. We divide the configuration space into  $M$  grid points. Then, we average the square of the absolute value of the difference between the exact solution and that obtained by the RSM on the grid points,

$$\delta_\psi^2 = \frac{\sum_{i,j=1}^M |\psi_{exact}(i, j) - \psi_N(i, j)|^2}{\sum_{i,j=1}^M |\psi_{exact}(i, j)|^2}, \quad \delta_E = \frac{|E_n^{exact} - E_n^{SM}|}{E_n^{exact}}. \quad (17)$$

In the above equation we have also shown the expression for  $\delta_E$ , for ease of reference. Figure 1 shows the ground state energy computed using SM for the fixed value of the  $N = 6$  as a function of  $L$ . Note the existence of the minimum point at the exact value of the eigenvalue. This point determines  $\hat{L}(6)$ . We repeat this procedure for a few other values of  $N$ . After plotting these values we can obtain an interpolating function  $\hat{L}(N)$  (Fig. 2). The optimization method introduce here is equivalent to the one introduced in Ref. [12], where inflection points determined the quantities  $\hat{L}(N)$ . Table 1 shows the complete results for the first 10 eigenvalues and eigenvectors for  $N = 22$ . Several points are note worthy here. First, note the outstanding accuracy of  $\delta_E \approx 10^{-15}$  for the ground state in particular, and the general good correspondence between  $\delta_E$  and  $\hat{\delta}_E$ . Also note the corresponding good accuracy for  $\delta_\psi$ , reported only for the non-degenerate cases. We did not calculate  $\delta_\psi$  for other cases because the outcome of the algorithm in each degenerate subspace causes an unpredictable linear combination of those wave

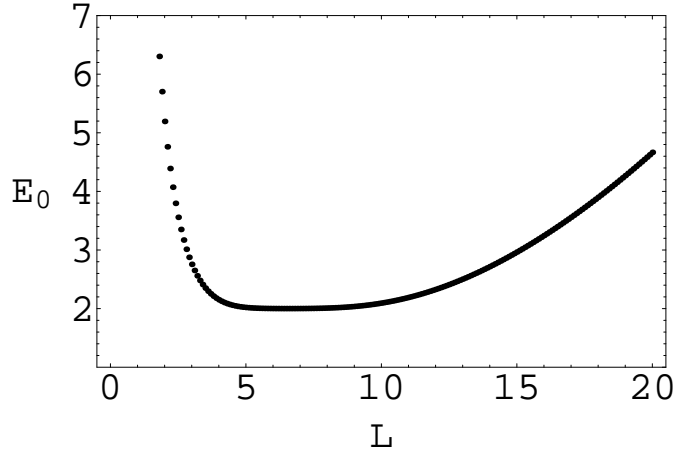


Figure 1: Ground state energy for 2D-SHO versus  $L$  for  $N = 6$ , using SM in units where  $\hbar\omega = 2$ . The position of the minimum determines  $\hat{L}(6)$ .

functions, which is equivalent to a whole rotation in that subspace. Hence the computation of  $\delta_\psi$  becomes a little complicated. Also note that the errors associated with wave functions symmetric in  $x$  and  $y$  are about one order of magnitude better than the asymmetric ones in the degenerate subspace, because we assumed this symmetry in our optimization procedure. In Fig. 3 we show a semi-log plot of the error for the ground state energy, obtained using RSM, in terms of  $N$ , all obtained using appropriate  $\hat{L}(N)$ . Note that the error falls off exactly exponentially as a function of  $N$ , a theoretical property common to all SM [13]. The exact matching of our computed error with this theoretical expectation is another positive sign for our method. In Fig. 4 we state the MATHEMATICA program for solving this problem, to emphasize how short our program is. We have only left out the the computation of  $\hat{L}(N)$ .

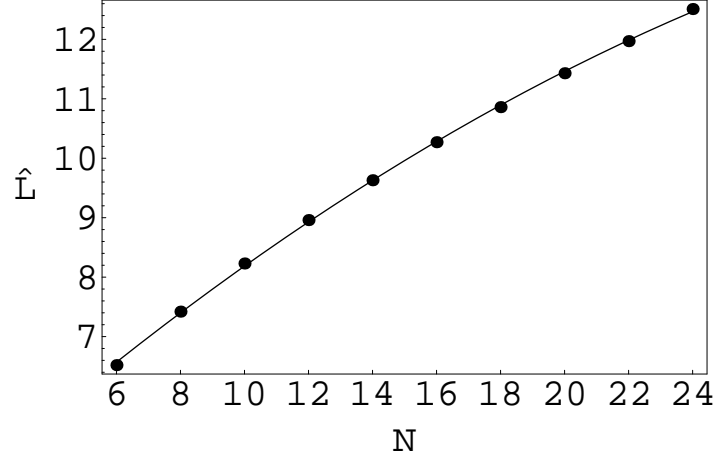


Figure 2: The dots represent the values of  $\hat{L}$  computed by the method described in the text for different values of  $N$ . The solid line represents the computed interpolation function  $\hat{L}(N)$ .

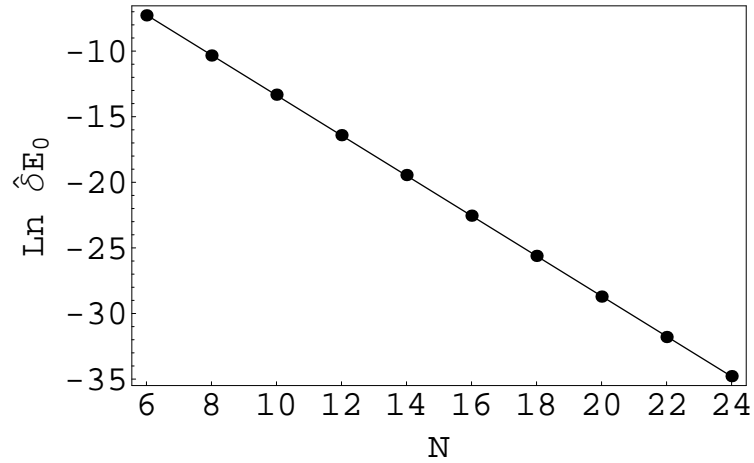


Figure 3: Semi-log plot of the error for the first eigenvalue of the 2D-SHO obtained by RSM using various number of basis functions.

$n_x, n_y$	$E_n^{exact}$	$E_n^{SM}$	$\delta_E$	$\hat{\delta}_E$	$\delta_\psi$
0,0	2.	2.0000000000000015572	$7.79 \times 10^{-15}$	$7.45 \times 10^{-15}$	$1.58 \times 10^{-8}$
0,1	4.	4.0000000000000278511	$6.96 \times 10^{-14}$	$6.68 \times 10^{-14}$	-
1,0	4.	4.0000000000000278512	$6.96 \times 10^{-14}$	$6.68 \times 10^{-14}$	-
1,1	6.	6.0000000000000541453	$9.02 \times 10^{-14}$	$8.63 \times 10^{-14}$	$1.90 \times 10^{-7}$
2,0	6.	6.0000000000018044778	$3.00 \times 10^{-12}$	$2.83 \times 10^{-12}$	-
0,2	6.	6.0000000000018044778	$3.00 \times 10^{-12}$	$2.83 \times 10^{-12}$	-
1,2	8.	8.000000000001830772	$2.29 \times 10^{-12}$	$2.16 \times 10^{-12}$	-
2,1	8.	8.000000000001830772	$2.29 \times 10^{-12}$	$2.16 \times 10^{-12}$	-
3,0	8.	8.00000000019999217	$2.50 \times 10^{-11}$	$2.38 \times 10^{-11}$	-
0,3	8.	8.00000000019999217	$2.50 \times 10^{-11}$	$2.38 \times 10^{-11}$	-
2,2	10.	10.00000000003607398	$3.61 \times 10^{-12}$	$3.41 \times 10^{-12}$	$8.23 \times 10^{-7}$
1,3	10.	10.00000000020025511	$2.00 \times 10^{-11}$	$1.90 \times 10^{-11}$	-
3,1	10.	10.00000000020025511	$2.00 \times 10^{-11}$	$1.90 \times 10^{-11}$	-
0,4	10.	10.00000000630282991	$6.30 \times 10^{-10}$	$5.90 \times 10^{-10}$	-
4,0	10.	10.00000000630282991	$6.30 \times 10^{-10}$	$5.90 \times 10^{-10}$	-
2,3	12.	12.00000000021802137	$1.81 \times 10^{-11}$	$1.73 \times 10^{-11}$	-
3,2	12.	12.00000000021802137	$1.81 \times 10^{-11}$	$1.73 \times 10^{-11}$	-
1,4	12.	12.00000000630309285	$5.25 \times 10^{-10}$	$4.24 \times 10^{-10}$	-
4,1	12.	12.00000000630309285	$5.25 \times 10^{-10}$	$4.24 \times 10^{-10}$	-
0,5	12.	12.00000003939548075	$3.28 \times 10^{-9}$	$3.08 \times 10^{-9}$	-
5,0	12.	12.00000003939548075	$3.28 \times 10^{-9}$	$3.08 \times 10^{-9}$	-
$\hat{L}(22)$	$\frac{1197}{100}$				

Table 1: The results for the first 21 eigenstates (out of 484) of the 2D-SHO in units where  $\hbar\omega = 2$ , using RSM with  $N = 22$ . That is we have used 484 basis functions and  $\hat{L}(22) = \frac{1197}{100}$ . Note that we obtain all the degeneracies and all with very good accuracy. Note that we have good correspondence between  $\delta_E$  and  $\hat{\delta}_E$ . The computation time was about 697.765 seconds for  $N = 22$  (using SetPrecision[... , 20] in MATHEMATICA) on a Pentium 2.4 GHz machine resulting in a precision of  $10^{-15}$  for the ground state energy, and it was 11.062 seconds for  $N = 18$  (using default double precision) resulting in a precision of  $10^{-12}$ .

```

NN = N;
U[x_, y_] := x^2 + y^2
L =  $\hat{L}$ ;
i = 1;
Nprecision = 50;
Do[
  {c1[i] = Integrate[ Sin[  $\frac{m \pi x}{L}$  ] Sin[  $\frac{n \pi y}{L}$  ] U[x - L/2, y - L/2] Sin[  $\frac{m1 \pi x}{L}$  ] Sin[  $\frac{n1 \pi y}{L}$  ],
    {x, 0, Lx}, {y, 0, Ly}], i = i + 1}, {m, 1, NN}, {n, 1, NN}, {m1, 1, NN}, {n1, 1, NN}];
Do[mat[m, n] = (2 / L) ^ 2 c1[ (m - 1) * NN ^ 2 + n] +
  KroneckerDelta[IntegerPart[ (m - 1) / NN + 1], IntegerPart[ (n - 1) / NN + 1]]
  KroneckerDelta[Mod[m - 1, NN] + 1, Mod[n - 1, NN] + 1]
  ((IntegerPart[ (n - 1) / NN + 1]  $\pi$  / L) ^ 2 + ((Mod[ (n - 1), NN] + 1)  $\pi$  / L) ^ 2),
  {m, 1, NN ^ 2}, {n, 1, NN ^ 2}];
Do[mat2[m, n] = SetPrecision[mat[m, n], Nprecision], {m, 1, NN ^ 2}, {n, 1, NN ^ 2}];
mat3 = Table[mat2[n, m], {m, 1, NN ^ 2}, {n, 1, NN ^ 2}];
Value = Eigenvalues[mat3]
Vec = Eigenvectors[mat3];

```

Figure 4: MATHEMATICA commands for computing the spectrum of the Hamiltonian  $H = p_x^2 + p_y^2 + U(x, y)$ , in units where  $\hbar = 1$ . The value for  $L$  in line 3 should be obtained by our optimization procedure as described in the text. Whenever possible we evaluate the integrals analytically, and replace the Integrate command by its results, to increase the precision and save time. This has been the case for the examples presented in this paper.

$n$	$E_n^{SM}$	$\hat{\delta}_E$
1	1.10822315780256	$1.19 \times 10^{-10}$
2	2.37863785124994	$1.16 \times 10^{-8}$
3	2.37863785124996	$1.16 \times 10^{-8}$
4	3.05608156130323	$2.06 \times 10^{-7}$
5	3.51495134040797	$1.12 \times 10^{-6}$
6	4.09348955687600	$9.38 \times 10^{-6}$
7	4.09348955687604	$9.38 \times 10^{-6}$
8	4.75298944936096	$9.32 \times 10^{-5}$
9	4.98538290136962	$1.75 \times 10^{-5}$
10	5.01127928161308	$4.59 \times 10^{-11}$
11	5.50103621623983	$7.92 \times 10^{-4}$
12	5.50103621623990	$7.92 \times 10^{-4}$
20	8.07437393671447	$6.64 \times 10^{-9}$
25	9.27305945794927	$3.36 \times 10^{-8}$
33	11.4718771513251	$7.24 \times 10^{-7}$
44	13.8662683175987	$8.33 \times 10^{-6}$
$\hat{L}(42)$	$\frac{1553}{100}$	

Table 2: The results for the eigenvalues ( $E_n^{SM}$ ) using RSM with  $N = 42$ , for the first 12 states and some other highly excited and interesting ones (as explained in the text) for the 2D-QCD Hamiltonian,  $p_x^2 + p_y^2 + x^2 y^2$ , in units where  $\hbar = 1$ .

## 4 An example which is not exactly solvable

The dimensionless and shifted Schrödinger equation for the example that we want to solve here is,

$$-\left(\frac{d^2\psi(x,y)}{dx^2} + \frac{d^2\psi(x,y)}{dy^2}\right) + \alpha (x - L/2)^2(y - L/2)^2\psi(x,y) = E\psi(x,y), \quad (18)$$

where  $\alpha$  is a positive constant. The potential in this example is sometimes called the 2D-QCD potential. This PDE is elliptic and not exactly solvable. Therefore, we use RSM to find its eigenvalues and eigenfunctions. In Table. 2 we have shown the eigenvalues for the first 12 states and some other highly excited ones ( $n = \{20, 25, 33, 44\}$ ). The latter were chosen for their unusually high accuracy due to their symmetric form, and the fact that we have chosen  $\hat{L}_x(N) = \hat{L}_y(N) = \hat{L}(N)$ . Figure 5 shows the ground state wave function. Note the slight over extension of the wave function in the  $x$  and  $y$  directions due to the particular form of the

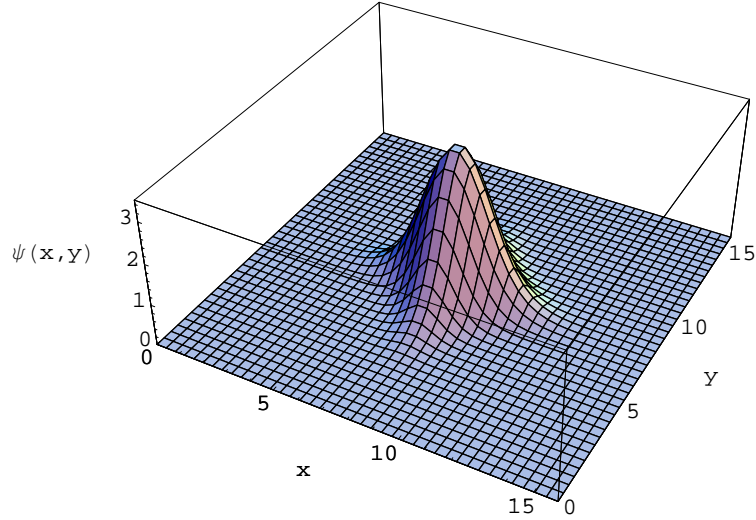


Figure 5: The wave function of the ground state of the 2D-QCD potential using  $N = 42$  and  $\hat{L}(42) = \frac{1553}{100}$ , in units where  $\hbar = 1$ .

potential. In Fig. 6 we show the wave functions for the second, forth, fifth, and forty forth eigenstates. The third eigenstate is not shown because it is degenerate with the second and can be obtained from it by 90 degree rotation. We have decided to show the forty forth state because we found it interesting and its highly symmetric form produces an unusually small error, as explained above.

## 5 Conclusions

We have extended the Refined Spectral Method to two dimensions and used it as an extremely accurate method for obtaining the energies and wave functions of the bound states of the two dimensional time-independent Schrödinger equation. In this method a finite basis is used for approximating the solutions. The refinement of the method is accomplished by calculating an optimized spatial domain for a given number of basis elements, denoted by  $\hat{L}(N)$ . The criteria for this optimization is to minimize the energy for one of the eigenstates, usually chosen to be the ground state. Note that our refined method is not quite equivalent to the Rayleigh-

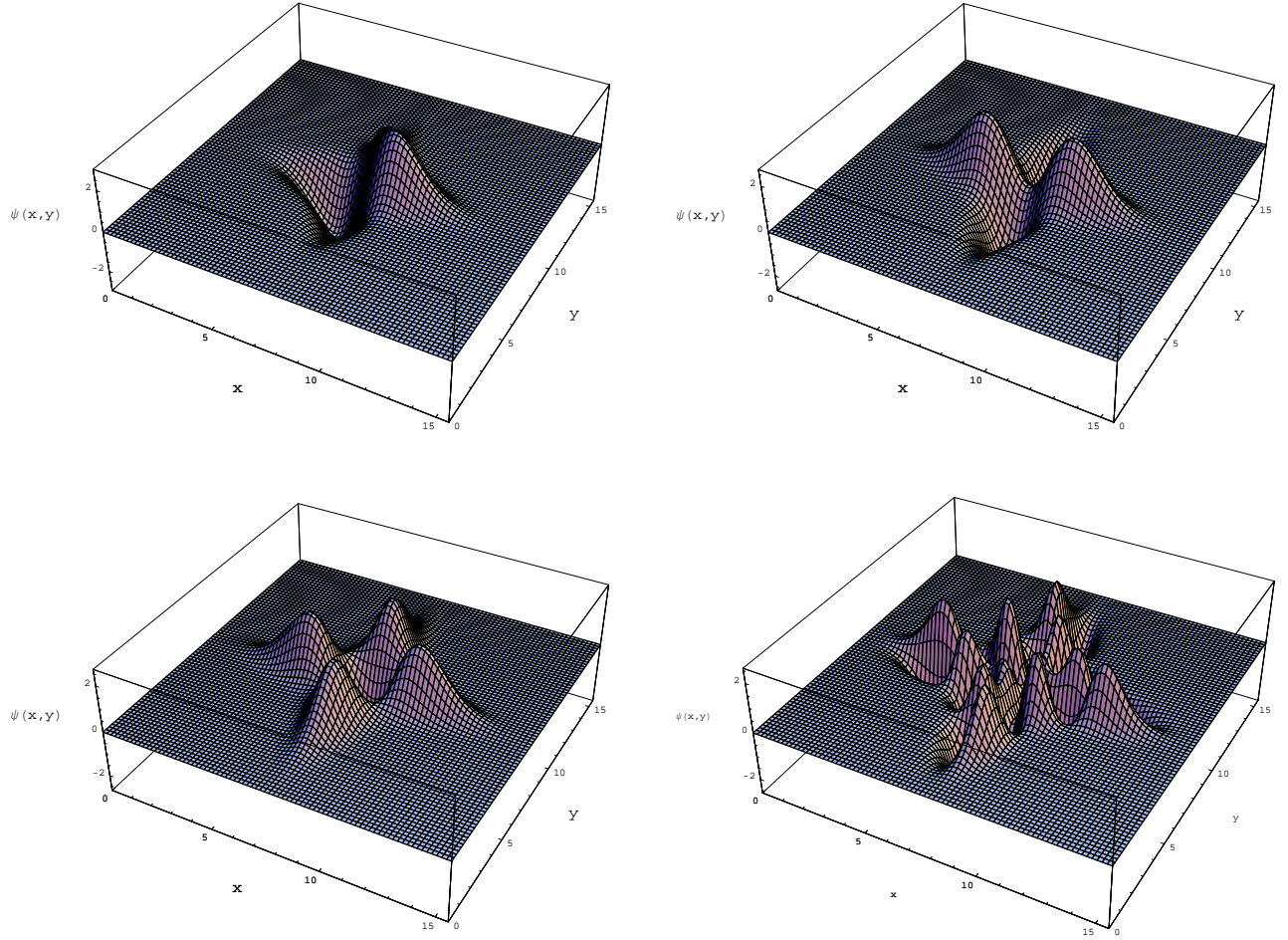


Figure 6: Some eigenfunctions of the 2D-QCD potential. Upper left: 2nd; Upper right 4th; Lower left: 5th, and lower right: 44th states, respectively. All the states are non-degenerate except the first one. Its degenerate wave function can be obtained by 90 degree rotation. The last one is shown because it is symmetrical, interesting, and has a relatively low error. Same parameters were used as for Fig. 5

Ritz variational method, in that we have combined the spectral method in which the wave function is expanded in an arbitrary basis with optimization of the spatial domain which is equivalent to adjusting the effective potential for the bound states. This effective potential for the case of the Fourier basis with confinement boundary condition is the actual potential plus the confining “walls” placed at the boundaries, which are separated by  $\hat{L}(N)$ . This refinement scheme usually improves the accuracy of SM drastically and this effect increases rapidly with  $N$ . We applied this method to an exactly solvable problem and easily found an extraordinarily good agreement with the exact solutions (errors of order  $10^{-15}$  with only 22 basis functions). This method is very simple, fast, extremely accurate in most cases, very robust, stable, and there is no need to specify the boundary conditions on the slopes. Most importantly, one can obtain the energies and the wave functions of as many of the bound states as desired with a single run of the algorithm. The generalization of this method to higher dimensional cases is straight forward.

## Acknowledgement

The Authors thank A. Turbinder for his useful suggestion regarding the QCD potential. This research has been supported by the office of research of Shahid Beheshti University under Grant No. 500/3787.

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